CCP4i - "Tricks and Tools"

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CCP4i - "Tricks and Tools"

- New in CCP4i 1.3.8
- Project Management Tools
 - Project Directories
 - Job Database & Project History
 - Electronic Notebook
 - Report External Tasks
- Data Harvesting
- File Viewers
 - Loggraph
 - MapSlicer
 - AstexViewer
- Installing new tasks
- Preferences

New in CCP4i 1.3.8

- New interfaces:
 - OASIS
 - ACORN
 - ANISOANL, TLSANL
 - BEAST
 - PROFESSS
 - ROTAMER
 - WHAT_CHECK (n.b. the program must currently be obtained from CMBI)
- New CCP4i-based application GET_PROT (aka SAPHIRE)
 - download & edit protein sequence data
- Updated interfaces and tools:
 - SCALA
 - Import Scaled Data task
 - Automatic reindexing facility in CAD task
 - Integrated viewers (MapSlicer, AstexViewer)
 - Task Interface Installer

Project Management Tools (1)

- Why Project Management?
 - Reminds you what you did six months ago
 - Helps keep track of multiple projects and associated data
 - Facilitates back-tracking (especially if things go wrong)
 - Helps when depositing results & writing your paper

• Project Directories

• Set up aliases for project directories in "Project & Project Directories" Window

• All data files relating to one crystallographic project should be in a single project directory

• Job Database & Project History

- Stores parameters used to run each task
- Records input, output and logfiles for each job
- Allows you to review parameters used
- Allows you to rerun a job with the same/modified parameters

Project Management Tools (2)

Access additional tools through the "Edit Job Data" option:

Title

Log

Out

Read/Edit Notebook

Edit Job Data

Enter Data for External Job

Electronic Notebook

• *Record information about a particular job for future reference*

• Edit Job Data

- Keep Job Database up-to-date
- Record changes e.g. of file locations

Report External Tasks

- Record runs of non-CCP4(i) programs plus associated files
- Keep project history complete

	CCP4I fileviewer 4_notebook.txt		
	Help		
cad	book for VORKSHOP job number 4 on 01 Feb 2001 11:41:32 4_cad.log e native vith NAD data		
wave	ined data from files with 5 datasets - native plus inflection point, low length remote,peak and high remote.		
r	- Edit Job Info		•
			Help
	Title Merge native with MAD data		C.
	current status FINISHED		
Ĩ	Control File WORKSHOP	Viev	v
	Log File WORKSHOP - 4 cad.log Browse	Viev	
	Input files for the job		
	Input File WORKSHOP - gere_nat_unique1.mtz Browse	Viev	v
	Input File WORKSHOP - gere_MAD_only.mtz Browse		, II
		Input File	
	Output files from the job	, ,	
	Report External Job Browse	Viev	v II
	Help 🛶 Add O	utput Filo	e "
ie 🛛			
VORKSHOP	Browse View		
RKSHOP 🚄	Browse View		
r the job			
	Edit list 🛁 Add Input File		
from the job			
	Edit list - Add Output File		
0,	ve&Exit Close		

Data Harvesting

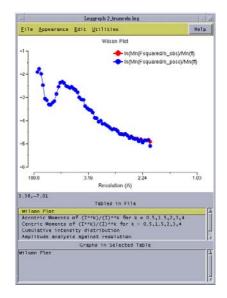
- Why is it useful?
 - Data is automatically collected in Harvest Files

• *The files can be deposited directly, reducing the amount of manual handling at deposition*

- What does it require?
 - Harvesting Project & Dataset names must be defined in MTZ file
 - Can be done at any entry point (e.g. "import" tasks) or via "Edit Project & Dataset Name" task
- How much work is it?
 - Switch harvesting on (or off) in Preferences or in individual tasks
 - That's all

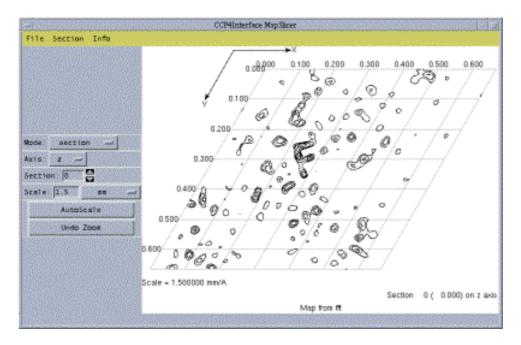
File Viewers (1)

- From within CCP4i:
 - View Files from Job: always uses default file viewer
 - View Any File: allows you to select from available viewers
- From Unix command line:
 - Use ccp4i -v <filename> to view a file in the default viewer
 - Useful for MTZ files (automatically runs mtzdump program to display header)
- HTML logfiles
 - Can be viewed as plain text or in HTML browser
- Loggraph
 - View tables and graphs in CCP4-formatted logfiles
 - Can also use loggraph <filename> at the command line



File Viewers (2)

- MapSlicer
 - Interactive viewer for map sections
 - Can view single sections or slabs on x, y or z axes
 - Special mode for viewing Harker sections
 - Can set this to be the default map viewer in "Preferences"



File Viewers (3)

• AstexViewer

module

- Java-based protein-ligand viewer
- Displays structures in electron density

to use XtalView - in "Model Building"

• Can be launched from "AstexViewer" task in Program List

	🖃 Netscape: AstexViewer: View mase coordinates in electron density 🍡 📋
	File Edit View Go Communicator Help
Launch AstezViewer Initial parameters from /ccpstaff/ccp4/pjx/DEVPR0J/CCP4_DATABASE/593_astex_viewer.de	Í 🎻 😂 3. 🏦 🧀 💩 💕 🕎
	Back Forward Reload Home Search Netscape Print Security 🚟
Job title View mase coordinates in electron density	📱 🋫 Bookmarks 🤹 Location: 📔 👘 🖓 🌍 What's Related
Launch hypertext browser to display html logfile automatically	#CCP4I PID 31271
Protein PDB files	AstexViewer: View rnase coordinates in electron density
PDB file 1 RNASE - mase.pdb Browse Mev	Proteins
Edit list Add input pdb file	rrotens ▼ mase.pdb
Ligand PDB files	
	Maps
Edit list	mase18_sfall1.map
Map files	
Map file 1 TEMPORARY rnase18_sfall1.map Browse View	
Edit list 🛹 Add input map file	+
Display Options	
Run - Save or Restore - Close	
Run Close Close	
alView/Xfit launcher	
	Documentation for the AstexViewer controls can be <u>found here</u> .
Also available for those who prefer	Please read and abide by the <u>Conditions of Use</u> .

100% 100% of 919K (at 3.1K/sec)

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Installing New Tasks

- Install task interfaces supplied for non-CCP4i programs •*e.g. ARP/wARP* 6.0
- Accessed from "System Administration" menu

• New tasks installed in main CCP4i area (available to all) or in user's "private" (i.e. \$HOME/.CCP4/..., available only to that user)

• Allows easy review, update (and de-installation) of currently installed task interfaces

-		Install (unin	ustall)CCP4i tasks			
					<u> 1999 - 1999</u>	Help
Run the Instal	lation Mana	jer to install a new t	ask 🛹			-
Perform aut	omatic 🚄	installation of tasks into	main CCP4i	🛶 area		
Install Packag	e Informatio	ņ				
Task archive	Full path	/ccpstaff/ccp4/pjx/E>	TERNAL_PROGS/a	rp_warp_6.0/ARP_	Browse	View
Name of pack	age: ARP_w	ARP_CCP4I	Version: 6.0			
Install Files		••••••		•••••		
All files in the	package wil	l be installed automatically				
Install Task Re	eterences					
Task referenc	es will be ac	lded automatically for this t	ask			
		Abbity		Close		

CCP4i Preferences

Set various useful things in the "Preferences":

- Default viewers for maps & PDB files
- Default locations and formats for map files
- Default Data Harvesting mode

😑 Set Preferences for CCP4Interface Initial parameters from /usr/users/pjx/.CCP4/unix/preferences.de 🍬 🗔							
Help							
Delete/Archive Files							
Default option in 'Delete/Archive Files' Delete temporary files 🛁							
File Selection 🕷							
In file selection list files by alphabetically by name 🔤							
Creating Maps							
By default create maps in CCP4 🛲 format in TEMPORARY 🛲 directory							
Mormalise maps output by Mapman for O program							
📑 In Refmac5 interface give output map names explicitly							
Default Viewers 🕷							
Set the default PDB viewer to TextViewer 🐭							
Set the default map viewer to MapSlicer (map sections) 🛁							
Data Harvesting 🛛 🖉							
By default Do not create harvest file 🐭							
j Create harvest directories to be private							
Maximum width of a row in the deposit file 60							
XML Output							
Save 🖂 Close							

Further Information ...

• Project Management Tools:

• "CCP4i as a Project Management Tool" - CCP4 Newsletter 38 (April 2000) http://www.ccp4.ac.uk/newsletter38/09_projman.html

• MapSlicer:

• "MAPSLICER: an interactive viewer for contoured map sections" - CCP4 Newsletter 39 (March 2001) http://www.ccp4.ac.uk/newsletter39/09 mapslicer.html

• What's New in CCP4i 1.3.8/Future Developments:

• "Developments with CCP4i" - CCP4 Newsletter 41 (October 2002) http://www.ccp4.ac.uk/newsletter41/02_ccp4i-oct02/ccp4ioct2002.html

• CCP4i Webpage:

• http://www.ccp4.ac.uk/ccp4i_main.html

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The End.

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